

Effective field theory description of topological crystalline insulators

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We propose a phenomenological theory for topological crystalline insulators with time reversal and C_4 symmetries. First, we introduce a fictitious space and transformation of electromagnetic field operators. This transformation leaves the speed of light unchanged but changes the elementary charge to $\sqrt{2}e$. Then we formulate the theory of topological crystalline insulators in terms of transformed fields in this fictitious space as 3D BF theory containing π -flux excitations. It is known that a 3D BF theory with half flux quantum excitations describes low energy properties of time reversal invariant insulators. By making an inverse transform we recover the effective field theory in original space. It turns out that this field theory contains quarter flux quantum excitations.

I. INTRODUCTION

In a recent paper¹, Fu showed that there are 3D topological band insulators characterized by a Z_2 index protected by time reversal and C_4 symmetries. These insulators have gapless surface states, 2D massless fermions with quadratic spectrum, only on one of their surfaces (the one which is perpendicular to the C_4 symmetry axis). Other surfaces of these insulators turn out to be gapped.

Three-dimensional time reversal invariant insulators²⁻⁴ are characterized by the following topological response,^{5,6} the axion term ($c = 1$)

$$\frac{\theta e^2}{2\pi h} \mathbf{E} \cdot \mathbf{B} \quad (1)$$

with $\theta = (2n - 1)\pi$ in the non-trivial phase. Since the axion term (1) is related to a surface quantum Hall effect with the conductivity $\frac{\theta}{2\pi} \frac{e^2}{h}$, and since the Hall conductivity of massless 2D fermions with quadratic spectrum is twice as bigger than that of massless 2D fermions with linear spectrum, one may expect that electromagnetic response of topological crystalline insulators of Ref.1 is given by an axion term with $\theta = 2\pi$. We show that this is indeed the case by employing the technique for computation of the axion term described in the paper 7.

There is a topological field theory description of 3D time reversal invariant insulators⁸ which is given by 3D BF theory

$$\mathcal{L}_{BF} = \frac{k}{4\pi} \varepsilon^{\mu\nu\rho\lambda} a_\mu \partial_\nu b_{\rho\lambda} + \frac{1}{2\pi} \varepsilon^{\mu\nu\rho\lambda} A_\mu \partial_\nu b_{\rho\lambda}$$

where $k = \frac{2}{2n-1}$. This theory can explain all of the main properties of 3D time-reversal invariant insulators: Z_2 -ness, axion term, gapless edge theory. One may wonder is there an analogous theory for crystalline insulators protected by point group symmetries.¹

In constructing such a theory one is faced with some difficulties which are clear already at this stage of discussion. One of them is related to the fact that C_4 symmetry of the underlying microscopic model can not enter the topological field theory in an explicit way and should be hidden. Second is related to the fact that an axion term with $\theta = 2\pi$ is equivalent to an axion term with $\theta = 0$ due to 2π periodicity,^{5,6,9,10} which makes it difficult to explain Z_2 -ness of topological crystalline insulators in the context of topological field theory.

In this paper, we construct a theory that allows to circumvent difficulties mentioned above. This theory explains Z_2 classification of topological crystalline insulators not in terms of original fields, but in terms of fields transformed to a fictitious space. It turns out that unit charge in this space is different from that of an electron charge and as a consequence it follows that 2π axion electrodynamics transforms to π axion electrodynamics. This is crudely how Z_2 classification is explained. This theory also contains traces of C_4 symmetry because it supports quarter flux quantum excitations.

II. COMPUTATION OF THE TOPOLOGICAL RESPONSE

Consider the following hamiltonian

$$H(k_x, k_y, k_z) = \hat{h}(k_x, k_y) \otimes \tau_z + M \cdot \mathbb{1} \otimes \tau_x - k_z \cdot \mathbb{1} \otimes \tau_y$$

where

$$\hat{h}(k_x, k_y) = \frac{k^2}{2m} + \frac{1}{2m_1}(k_x^2 - k_y^2) \cdot \hat{\sigma}_z + \frac{1}{m_2}k_x k_y \cdot \hat{\sigma}_x \quad (2)$$

If $M > 0$ for $z > 0$ then (in the τ space) z -dependence of the wavefunction is

$$\psi = \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-Mz}$$

Analogously, if $M < 0$ for $z < 0$ then

$$\psi = \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{|M|z}$$

This means that there is a 2D massless chiral fermion with quadratic spectrum (2) localized near the surface which is perpendicular to the symmetry axis and which separates two models with different sign of mass M .

There are two symmetries of the hamiltonian, time reversal operation T which coincides with complex conjugation K , and C_4 rotation in the (k_x, k_y) plane $U = \hat{\sigma}_y \otimes 1$, $(UT)^2 = -1$:

$$T^{-1}H(k_x, k_y, k_z)T = H(-k_x, -k_y, -k_z), \quad U^{-1}H(k_x, k_y, k_z)U = H(k_y, -k_x, k_z)$$

We will compute the axion term assuming that $\hat{h}(k_x, k_y) = \frac{1}{2m_1}(k_x^2 - k_y^2) \cdot \hat{\sigma}_z + \frac{1}{m_2}k_x k_y \cdot \hat{\sigma}_x$, where $m_1 = m_2$, using the approach given in the appendix of Ref. 7. Calculation can be easily generalized for unequal masses $m_1 \neq m_2$, but unfortunately we could not do the calculation for generic h , Eq. (2). Lagrangian in the euclidean space-time is

$$\bar{\psi}(\gamma_\mu d_\mu - M)\psi$$

where

$$\gamma_0 = \mathbb{1} \otimes \hat{\tau}_x, \quad \gamma_1 = \sigma_z \otimes \tau_y, \quad \gamma_2 = \sigma_x \otimes \tau_y, \quad \gamma_3 = \mathbf{1} \otimes \tau_z, \quad \gamma_5 = \sigma_y \otimes \tau_y = \gamma_0 \gamma_1 \gamma_2 \gamma_3$$

$$d_0 = \partial_t + iA_0, \quad d_1 = \frac{i}{2m}(k_y^2 - k_x^2), \quad d_2 = -\frac{i}{2m}(k_x k_y + k_y k_x), \quad d_3 = \partial_z + iA_z, \quad k_{x,y} = \partial_{x,y} + iA_{x,y}$$

$M \rightarrow Me^{i\gamma_5}$ interpolates between hamiltonians with different sign of mass when α varies from 0 to π , violating time reversal symmetry for intermediate values of α . If α slowly varies in space such that there is a domain wall on which the mass M flips the sign, then the action on one of the sides of the domain wall will contain an additional term with respect to the action on the opposite side. This additional term is an anomaly due to the change of the Jacobian under the transformation $\psi' = e^{i\alpha\gamma_5/2}\psi$. This anomaly can be computed by a proper regularization, using Fujikawa method, and is given by

$$i\pi \int \frac{d^4 k}{(2\pi)^4} \text{tr}\{\gamma_5 f[\langle k | (\gamma_\mu d_\mu)^2 / M^2 | k \rangle]\} \quad (3)$$

where the function $f(s)$ satisfies the requirements

$$f(0) = 1, \quad f(\infty) = 0, \quad sf'(s) = 0 \quad \text{when} \quad s = 0, \infty$$

It is easy to show that $(\gamma_\mu d_\mu)^2 = d_\mu d_\mu + 1/4[\gamma_\mu, \gamma_\nu][d_\mu, d_\nu]$. Since $\text{tr}\{\gamma_5[\gamma_\mu, \gamma_\nu][\gamma_\rho, \gamma_\sigma]\} = 16\varepsilon_{\mu\nu\rho\sigma}$, in the absence of the gauge fields, $A_\mu = 0$, one obtains $\langle k | -(\gamma_\mu d_\mu)^2 | k \rangle = k_0^2 + k_z^2 + (k_x^2 + k_y^2)^2/4m^2$. To obtain a non-zero result in (3) in the limit $M \rightarrow \infty$ we need to expand f up to the second order in $[\gamma_\mu, \gamma_\nu][d_\mu, d_\nu]/M^2$ and retain the terms in $[d_\mu, d_\nu][d_\rho, d_\sigma]$ which contain the operators ∂_x^2 and ∂_y^2 . Namely, the terms that should be retained are

$$[d_0, d_3] = iE_z, \quad [d_1, d_2] = \frac{i}{m^2}B_z(\partial_x^2 + \partial_y^2) + \dots \quad (4)$$

$$[d_0, d_1] = \frac{1}{m}(E_y \partial_y - E_x \partial_x) + \dots, \quad [d_3, d_2] = \frac{1}{m}(B_y \partial_y - B_x \partial_x) + \dots \quad (5)$$

$$[d_0, d_2] = \frac{1}{m}(E_x \partial_y + E_y \partial_x) + \dots, \quad [d_3, d_1] = -\frac{1}{m}(B_y \partial_x + B_x \partial_y) + \dots \quad (6)$$

Then (3) becomes

$$i\pi \int \frac{d^4 k}{(2\pi)^4} \cdot 4 \cdot \frac{1}{M^4} \langle k | \{ [d_0, d_1][d_2, d_3] - [d_0, d_2][d_1, d_3] + [d_0, d_3][d_1, d_2] \} | k \rangle f''(s) = i\pi \int \frac{d^4 k}{(2\pi)^4} \cdot 4 \cdot \frac{1}{M^4 m^2} \cdot (\mathbf{BE}) \cdot (k_x^2 + k_y^2) f''(s)$$

where $s = k_0^2 + k_z^2 + (k_x^2 + k_y^2)/4m^2$. Calculating the integral, which does not depend on the specific choice of the function f , we get the axion term $i \frac{\theta}{2\pi h} (\mathbf{BE})$ with $\theta = 2\pi$.

III. TRANSFORMATION OF ELECTROMAGNETIC FIELD

In this section we introduce a fictitious space (denoted in the following by $\tilde{}$) and a transformation of electromagnetic field which is motivated by the previous discussion, Eqs.(4–6). The aim is to reformulate the theory in this fictitious space and in terms of transformed electromagnetic field operators.

It is more convenient to work in momentum space. Momentum operators in $\tilde{}$ space are given by

$$K_x = \frac{k_x^2 - k_y^2}{k_\perp}, \quad K_y = \frac{2k_x k_y}{k_\perp}, \quad K_z = k_z \quad (k_y > 0) \quad (7)$$

and with reverse sign for $k_y < 0$. From this definition one can see that the absolute value of the momentum does not change since $K_x^2 + K_y^2 = k_\perp^2$, and that the vector \mathbf{K} covers $\tilde{}$ momentum space twice. This means that electromagnetic field operators in $\tilde{}$ space split into two fields (generally, every field that can be transformed into $\tilde{}$ space will split into two fields). We will divide \mathbf{k}_\perp plane into two regions: 1) $\text{sgn} k_x = \text{sgn} k_y$ ($l = 1$) and 2) $\text{sgn} k_x = -\text{sgn} k_y$ ($l = 2$). The relation between \mathbf{k} and \mathbf{K} integrations is given by

$$2 \int d^3 k = \sum_{l=1,2} \int d^3 K \quad (8)$$

Scalar field in $\tilde{}$ space is defined according to relations

$$\tilde{\phi}^{(1)}(\mathbf{K}) = \frac{\phi(\mathbf{k})}{\sqrt{2}}, \quad (k_x, k_y > 0); \quad \tilde{\phi}^{(2)}(\mathbf{K}) = \frac{\phi(\mathbf{k})}{\sqrt{2}}, \quad (-k_x, k_y > 0) \quad (9)$$

and $\tilde{\phi}^{(l)}(-\mathbf{K})$ is defined as complex conjugate of Eqs.(9), such that in accordance with (8) we have

$$\int \phi(\mathbf{k}) \phi(-\mathbf{k}) d^3 k = \sum_{l=1,2} \int \tilde{\phi}^{(l)}(\mathbf{K}) \tilde{\phi}^{(l)}(-\mathbf{K}) d^3 K$$

Transformation formulas for vector potential must be consistent with Eq. (9). They are defined as follows

$$\tilde{A}_x^{(l)}(\mathbf{K}) = \frac{k_x A_x(\mathbf{k}) - k_y A_y(\mathbf{k})}{\sqrt{2} k_\perp}, \quad \tilde{A}_y^{(l)}(\mathbf{K}) = \frac{k_y A_x(\mathbf{k}) + k_x A_y(\mathbf{k})}{\sqrt{2} k_\perp}, \quad \tilde{A}_z^{(l)}(\mathbf{K}) = \frac{A_z(\mathbf{k})}{\sqrt{2}} \quad (10)$$

and $\tilde{\mathbf{A}}^{(l)}(-\mathbf{K})$ as complex conjugate of (10). One can see from Eq. (10) that when vector potential in original space is a pure gauge, then it is pure gauge also in $\tilde{}$ space, which is quite reasonable. Transformation formulas for electric and magnetic fields can be obtained by substituting (9) and (10) into equations $\tilde{E}_i = -\partial_t \tilde{A}_i - \partial_i \tilde{\phi}$, $\tilde{H}_i = \varepsilon_{ijk} \partial_j \tilde{A}_k$. The result is that $\tilde{\mathbf{E}}$ and \mathbf{E} , $\tilde{\mathbf{H}}$ and \mathbf{H} are related to each other exactly by the same formulas as $\tilde{\mathbf{A}}$ and \mathbf{A} , Eq. (10), and $\tilde{\mathbf{E}}^{(l)}(-\mathbf{K})$, $\tilde{\mathbf{H}}^{(l)}(-\mathbf{K})$ by their complex conjugates:

$$\tilde{E}_x^{(l)}(\mathbf{K}) = \frac{k_x E_x(\mathbf{k}) - k_y E_y(\mathbf{k})}{\sqrt{2} k_\perp}, \quad \tilde{E}_y^{(l)}(\mathbf{K}) = \frac{k_y E_x(\mathbf{k}) + k_x E_y(\mathbf{k})}{\sqrt{2} k_\perp}, \quad \tilde{E}_z^{(l)}(\mathbf{K}) = \frac{E_z(\mathbf{k})}{\sqrt{2}} \quad (11)$$

$$\tilde{H}_x^{(l)}(\mathbf{K}) = \frac{k_x H_x(\mathbf{k}) - k_y H_y(\mathbf{k})}{\sqrt{2} k_\perp}, \quad \tilde{H}_y^{(l)}(\mathbf{K}) = \frac{k_y H_x(\mathbf{k}) + k_x H_y(\mathbf{k})}{\sqrt{2} k_\perp}, \quad \tilde{H}_z^{(l)}(\mathbf{K}) = \frac{H_z(\mathbf{k})}{\sqrt{2}} \quad (12)$$

It is also possible to incorporate source terms (current j^μ) into the theory, transformation properties of which are analogous to (9),(10).

One of the consequences of Eqs. (11) and (12) is that scalar products in two spaces differ by a factor of 2. For instance, $\tilde{\mathbf{E}}(\mathbf{K})\tilde{\mathbf{E}}(-\mathbf{K}) = \mathbf{E}(\mathbf{k})\mathbf{E}(-\mathbf{k})/2$, and analogous formulas are true also for the scalar product of the pairs $\tilde{\mathbf{H}}(\mathbf{K})$ and $\tilde{\mathbf{H}}(-\mathbf{K})$, $\tilde{\mathbf{E}}(\mathbf{K})$ and $\tilde{\mathbf{H}}(-\mathbf{K})$. This leads to equalities

$$\int \mathbf{E}^2 d^3x = \sum_{l=1,2} \int [\tilde{\mathbf{E}}^{(l)}]^2 d^3x, \quad \int \mathbf{H}^2 d^3x = \sum_{l=1,2} \int [\tilde{\mathbf{H}}^{(l)}]^2 d^3x$$

which mean, in particular, that lagrangian density of electromagnetic field does not change its form and, therefore, \tilde{A} is a true electromagnetic potential in $\tilde{\sim}$ space. Electric and magnetic fields (11) and (12) defined in this way satisfy Maxwell's equations with the same speed of light c .

Coulomb gauge condition $\mathbf{k}\mathbf{A}(\mathbf{k}) = 0$ transforms to $\mathbf{K}\tilde{\mathbf{A}}(\mathbf{K}) = 0$. So, it can be checked by direct computation that the commutation relations¹¹ $[E_i(\mathbf{k}), A_j(-\mathbf{k}')] = 4\pi i \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \cdot (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}')$, which are satisfied in quantum theory in the Coulomb gauge, are transformed to $[\tilde{E}_i^{(l)}(\mathbf{K}), \tilde{A}_j^{(l')}(-\mathbf{K}')] = 4\pi i \left(\delta_{ij} - \frac{K_i K_j}{K^2} \right) \cdot (2\pi)^3 \delta(\mathbf{K} - \mathbf{K}') \delta_{ll'}$. This means that transformation formulas (10) are correctly defined also in quantum theory.

To see how the axion term transforms one needs to consider θ varying in space. If $\theta = \theta(z)$ then, rewriting the integral in momentum space, it can be shown that

$$\int \theta(z) \mathbf{E} \mathbf{H} d^3x = \sum_l \int \theta(z) \tilde{\mathbf{E}}^{(l)} \tilde{\mathbf{H}}^{(l)} d^3x$$

So one can write

$$\int_M \mathbf{E} \mathbf{H} = \sum_l \int_{\tilde{M}} \tilde{\mathbf{E}}^{(l)} \tilde{\mathbf{H}}^{(l)} \quad (13)$$

IV. SOME OTHER PROPERTIES OF THE FICTITIOUS ELECTRODYNAMICS

One of the consequences of Eq. (9) is that the scalar potential of a static point charge q , $\phi(\mathbf{k}) = 4\pi q/k^2$, becomes $\tilde{\phi}(\mathbf{K}) = 4\pi \tilde{q}/K^2$, $\tilde{q} = q/\sqrt{2}$, i.e. scalar potential of a static point charge $q/\sqrt{2}$. More generally, a simple correspondence can be made between electric field distributions in the two spaces when the field configuration has axial symmetry. However, this does not mean that elementary charge in $\tilde{\sim}$ space \tilde{e} is given by $1/\sqrt{2}$ units of electronic charge.

In the same way, one can obtain the transformation $q_m \rightarrow \tilde{q}_m = q_m/\sqrt{2}$, $\phi \rightarrow \tilde{\phi} = \phi/\sqrt{2}$ for a magnetic pole q_m and a magnetic flux vertex ϕ parallel to z axis.

There is one more configuration which has simple transformation properties, a skyrmion. Consider the simplest skyrmion in 2+1D

$$\phi_0(r, \varphi) = \cos f(r), \quad \phi_x(r, \varphi) = \sin f(r) \cos \varphi, \quad \phi_y(r, \varphi) = \sin f(r) \sin \varphi \quad (14)$$

This can be written in more convenient form as

$$\phi_0 = \cos f(r), \quad \phi_x = \partial_x \int_0^r \sin f(r') dr', \quad \phi_y = \partial_y \int_0^r \sin f(r') dr'.$$

Transformation formulas for ϕ_i are analogous to (10) (we drop the factor $\frac{1}{\sqrt{2}}$ because it does not affect the final result), and in coordinate space we obtain

$$\tilde{\phi}_0^{(l)}(r, \varphi) = \cos f(r), \quad \tilde{\phi}_x^{(l)}(r, \varphi) = \sin f(r) \cos \varphi, \quad \tilde{\phi}_y^{(l)}(r, \varphi) = \sin f(r) \sin \varphi, \quad l = 1, 2, \quad (15)$$

where r and φ are polar coordinates in $\tilde{\sim}$ space.

When a skyrmion is coupled to a doublet of two-component fermions through the interaction lagrangian $g\sigma_z(\phi\hat{\tau})$, it acquires quantum numbers, charge and spin.¹²⁻¹⁴ For the skyrmion coupled to Dirac fermions induced fermion current is given by the topological current of the skyrmion (we put number of flavours $N_f = 1$)

$$J_\mu = \frac{1}{8\pi} \varepsilon_{\mu\nu\lambda} \varepsilon_{ijk} n_i \partial_\nu n_j \partial_\lambda n_k \quad (16)$$

where $n_i = \phi_i/|\phi|$, and spin is determined by the Hopf term

$$S_{Hopf} = i\pi \int d^3x J^\mu C_\mu \quad (17)$$

where the gauge field C_μ is related to the current through the relation $J_\mu = \varepsilon_{\mu\nu\lambda} \partial_\nu C_\lambda$. Charge is given by the temporal component of (16)

$$Q = \int d^2x \frac{1}{4\pi} \varepsilon_{ijk} n_i \partial_x n_j \partial_y n_k$$

The skyrmion configuration (14) has charge $Q = e$ and spin $s = \frac{1}{2}$. We note that spin can not be treated according to quasiclassical equations (10). Correct quasiclassical treatment of the spin of a skyrmion is as in Refs.15–17.

However, we are interested in skyrmions in fermion models with quadratic band touching. These were studied in¹⁸ and the main result can be formulated as the doubling of quantum numbers compared to fermions with linear spectrum. Thus, we have that the skyrmion (14) coupled to fermions with quadratic spectrum has charge $Q = 2e$ and spin $s = 1$. This is analogous to doubling of the θ term that we have found in Sec. II. After transformation to $\tilde{\sim}$ space, the Hopf term $S_{Hopf} = 2i\pi \int d^3x J^\mu C_\mu$ of such a skyrmion will be equally distributed between skyrmions (15): $S_{Hopf} = \tilde{S}_{Hopf}^{(1)} + \tilde{S}_{Hopf}^{(2)}$, $\tilde{S}_{Hopf}^{(l)} = i\pi \int d^3x \tilde{J}^\mu \tilde{C}_\mu$, where $\tilde{J}_\mu = \frac{1}{8\pi} \varepsilon_{\mu\nu\lambda} \varepsilon_{ijk} \tilde{n}_i \tilde{\partial}_\nu \tilde{n}_j \tilde{\partial}_\lambda \tilde{n}_k$, $\tilde{n}_i = \tilde{\phi}_i/|\tilde{\phi}|$ (we note that fermionic charge current is $\tilde{j}_\mu = \sqrt{2}e \tilde{J}_\mu$). This means that skyrmions in $\tilde{\sim}$ space will have half of the spin of the skyrmion in original space. In the case under consideration, their spin is $\frac{1}{2}$, i.e. they are fermions.

We saw that the correspondence $S_{Hopf} = \tilde{S}_{Hopf}^{(1)} + \tilde{S}_{Hopf}^{(2)}$ holds for the skyrmions (14) and (15), but it can be shown that it is more general. One can see that $\tilde{\phi}_i$ depends continuously on ϕ_i . If we continuously deform ϕ_i then S_{Hopf} does not change, since it is topological invariant. Analogously, $\tilde{S}_{Hopf}^{(l)}$ does not change under continuous deformations of $\tilde{\phi}_i$. So $S_{Hopf} = \tilde{S}_{Hopf}^{(1)} + \tilde{S}_{Hopf}^{(2)}$ remains valid for continuous deformations of the skyrmions (14) and (15).

Thus, we have established that transformation of spin-1 bosonic skyrmions with electric charge $2e$ to $\tilde{\sim}$ space results in two different types of spin- $\frac{1}{2}$ fermions each having charge $\sqrt{2}e$. Suppose that we interpret this as $\tilde{e} = \sqrt{2}e$. Since θ term is proportional to the square of elementary charge, this means that the value of the θ -angle in $\tilde{\sim}$ space is two times smaller than in original space. This idea is pursued further in the next section from different point of view.

Now we consider an example for illustration, an axially symmetric charge distribution $\rho(r)$ rotating around the symmetry axis z with small angular velocity ω ($\omega a \ll c$, a is characteristic size in transverse direction). We have $j_x = -\omega \partial_y g(r)$, $j_y = \omega \partial_x g(r)$, $j_z = 0$, where $g(r) = \int_0^r \rho(r') dr'$. Transformation to $\tilde{\sim}$ space gives $\tilde{\rho}^{(l)}(r) = \frac{1}{\sqrt{2}} \rho(r)$, $\tilde{j}_x^{(l)} = -\omega \tilde{\partial}_y \tilde{g}(r)$, $\tilde{j}_y^{(l)} = \omega \tilde{\partial}_x \tilde{g}(r)$, $l = 1, 2$ where $\tilde{g}(r) = \int_0^r \tilde{\rho}(r') dr'$. This means that angular velocity in $\tilde{\sim}$ space is the same as in original space. In particular, rotation around z axis in original space of an axially symmetric configuration results in rotation by the same angle in $\tilde{\sim}$ space. Wavefunction of a bosonic skyrmion ($S_z = 1$) acquires phase factor 2π after 2π rotation in original space. However, in $\tilde{\sim}$ space we have phase factor π for each sector l , such that $2\pi = \pi + \pi$. Together with the fact that spinor ($S_z = 1/2$) acquires phase factor π after 2π rotation, this means that the skyrmion (15) in $\tilde{\sim}$ space is a fermion.

V. BF THEORY

In this section, after briefly reviewing 3D BF theory, we turn to the study of the following possibility that a system in $\tilde{\sim}$ space is described by a 3D BF theory with $k = 2$. We will show that transformation of electromagnetic field operators defined in section III is consistent with quantization of charge in $\tilde{\sim}$ space in $\sqrt{2}$ units of elementary charge. This in turn means that a $\theta = 2\pi$ axion electrodynamics becomes a $\theta = \pi$ axion electrodynamics in $\tilde{\sim}$ space. Transformation of this model to the original space gives a BF theory with $k = 4$ and we argue that this is an effective field theory for topological crystalline insulators with C_4 symmetry.

A. Review of 3D BF theory

3D BF theory contains two statistical fields a_μ and $b_{\mu\nu}$ coupled to quasiparticle and vortex currents

$$\mathcal{L}_{BF} = \frac{k}{4\pi} \varepsilon^{\mu\nu\rho\lambda} a_\mu \partial_\nu b_{\rho\lambda} + j^\mu a_\mu + \frac{1}{2} \Sigma^{\mu\nu} b_{\mu\nu}$$

The first term imposes non-trivial statistics between quasiparticles and vortices: when a quasiparticle j is rotated around a vortex Σ the full wavefunction of the system changes by a phase $\frac{2\pi}{k}$.¹⁹ In the absence of quasiparticles and vortices lagrangian can be written as

$$L_{BF} = \frac{k}{2\pi} \int d^3x a_i \dot{b}_i + a_0 (\partial_i b_i) + b_{0i} (\varepsilon_{ijk} \partial_j a_k)$$

where $b_i = \frac{1}{2} \varepsilon_{ijk} b_{jk}$. Integrating out a_0 and b_{0i} gives the constraints $\partial_i b_i = 0$ and $\varepsilon_{ijk} \partial_j a_k = 0$ which can be resolved on a torus by taking²⁰

$$a_i = \frac{\bar{a}_i}{L_i} + \partial_i \Lambda, \quad b_i = \frac{\bar{b}_i}{S_i} + \varepsilon_{ijk} \partial_j \zeta_k$$

where Λ and ζ are periodic functions, $L_i S_i$ is the volume of the system. The final lagrangian contains only \bar{a}_i and \bar{b}_i

$$L_{BF} = \frac{k}{2\pi} \bar{a}_i \partial_t \bar{b}_i$$

It is possible to construct gauge invariant quantities from \bar{a}_i and \bar{b}_i , Wilson loops and Wilson surfaces²¹

$$\mathcal{A}_i = e^{ie\bar{a}_i}, \quad \mathcal{B}_i = e^{i\phi_0 \bar{b}_i}$$

This means that $\bar{a}_i \equiv \bar{a}_i + \frac{2\pi}{e}$ and $\bar{b}_i \equiv \bar{b}_i + \frac{2\pi}{\phi_0}$ which is a manifestation of quasiparticle and vortex number quantization.

B. Effective field theory description of topological crystalline insulators

a and A appear in the BF theory in the combination $a + A$, so a transforms in the same way as the electromagnetic potential. However, \bar{a} on a compact surface should be treated differently because it is not possible to define $\tilde{\bar{a}}$ as the $K \rightarrow 0$ limit of the continuous expression. Instead we write

$$\frac{k}{2\pi} \bar{a}_i \partial_t \bar{b}_i = \frac{\tilde{k}}{2\pi} \sum_l \tilde{\bar{a}}_i^{(l)} \partial_t \tilde{\bar{b}}_i^{(l)}, \quad \tilde{k} = \frac{k}{2} \quad (18)$$

where $\tilde{\bar{a}}_i^{(1)} = \tilde{\bar{a}}_i^{(2)} = \bar{a}_i/\gamma$, $\tilde{\bar{b}}_i^{(1)} = \tilde{\bar{b}}_i^{(2)} = \gamma \bar{b}_i$ for some numeric constant γ . Since Wilson loops and Wilson surfaces in $\tilde{\sim}$ space are given by

$$\tilde{\mathcal{A}}_i = e^{i\tilde{e}\tilde{\bar{a}}_i}, \quad \tilde{\mathcal{B}}_i = e^{i\tilde{\phi}_0 \tilde{\bar{b}}_i}, \quad \tilde{e}\tilde{\phi}_0 = e\phi_0$$

it follows that $\tilde{e} = \gamma e$. Thus $\tilde{\bar{b}}_i = \gamma^2 \cdot \bar{b}_i/\gamma$, which means that transformation formulas for $\tilde{\bar{b}}$ are given by that of $\tilde{\bar{a}}$ with an extra factor of γ^2 , such that

$$\gamma^2 \frac{\tilde{k}}{2\pi} \int_M a_i \partial_t b_i = \frac{\tilde{k}}{2\pi} \sum_l \int_{\tilde{M}} \tilde{\bar{a}}_i^{(l)} \partial_t \tilde{\bar{b}}_i^{(l)} \quad (19)$$

For the two Eqs.(18) and (19) to be consistent with each other γ must be equal to $\sqrt{2}$. This means that $\tilde{e} = \sqrt{2}e$. The difference between transformation of a and b can be viewed as the consequence of charge-flux duality, since transformation formulas for $\tilde{\bar{a}}$ ($\tilde{\bar{b}}$) differ from that of momentum K by additional factor $1/\sqrt{2}$ ($\sqrt{2}$).

The full Lagrangian in $\tilde{\sim}$ space together with time-reversal symmetry breaking surface terms is given by the expression ($\tilde{k} = 2$)

$$\sum_l \int_{\tilde{M}} \frac{1}{2\pi} \varepsilon^{\mu\nu\rho\lambda} \tilde{\bar{a}}_\mu^{(l)} \tilde{\partial}_\nu \tilde{\bar{b}}_{\rho\lambda}^{(l)} + \frac{1}{2\pi} \varepsilon^{\mu\nu\rho\lambda} \tilde{\bar{A}}_\mu^{(l)} \tilde{\partial}_\nu \tilde{\bar{b}}_{\rho\lambda}^{(l)} + \frac{\tilde{e}^2}{8\pi} \varepsilon^{\mu\nu\rho\lambda} \tilde{\partial}_\mu \tilde{\bar{a}}_\nu^{(l)} \tilde{\partial}_\rho \tilde{\bar{A}}_\lambda^{(l)} \quad (20)$$

Lagrangian (20) is two copies of the model that was proposed in the Ref. 8 as an effective field theory for 3D topological insulators. Transformation of the model (20) to the original space gives a model with the Lagrangian density ($k = 4$)

$$\mathcal{L}_{TCI} = \frac{1}{\pi} \varepsilon^{\mu\nu\rho\lambda} a_\mu \partial_\nu b_{\rho\lambda} + \frac{1}{\pi} \varepsilon^{\mu\nu\rho\lambda} A_\mu \partial_\nu b_{\rho\lambda} + \frac{e^2}{4\pi} \varepsilon^{\mu\nu\rho\lambda} \partial_\mu a_\nu \partial_\rho A_\lambda \quad (21)$$

An interesting consequence of Eq.(21) is that vortex excitations in this model carry $\pi/2$ -flux, i.e. quarter flux quantum. This can be associated with C_4 symmetry, since due to C_4 symmetry of the microscopic model it is expected that quarter flux quantum must play a special role in the theory.

Transformation of \tilde{A} , \tilde{a} and \tilde{b} under time-reversal is the same as in original space: $(\tilde{A}_0, -\tilde{A}_i)$, $(\tilde{a}_0, -\tilde{a}_i)$ and $(-\tilde{b}_0, \tilde{b}_i)$ after time reversal, so the action (21) is time-reversal invariant. C_4 rotation in original space interchanges the sectors with $l = 1$ and $l = 2$ with each other.

If one integrates out a and b from Eq. (21) then the remaining term is a 2π axion term. Eq. (13), together with the fact that unit charge in $\tilde{}$ space is $\tilde{e} = \sqrt{2}e$, gives that

$$\frac{e^2\theta}{2\pi\hbar} \int_M \mathbf{E}\mathbf{H} = \frac{\tilde{e}^2\tilde{\theta}}{2\pi\hbar} \sum_l \int_{\tilde{M}} \tilde{\mathbf{E}}\tilde{\mathbf{H}}, \quad \tilde{\theta} = \frac{\theta}{2}$$

Thus a $\theta = 2\pi$ axion term transforms into two copies of $\tilde{\theta} = \pi$ axion terms. These two copies are different, because they involve Fourier components of electromagnetic field with different momenta. So one can not combine these two BF theories into a single BF theory with $\tilde{\theta} = 2\pi$. These two theories should be treated as independent unless there are other terms mixing them with each other.

Z_2 classification of topological crystalline insulators can be explained as it is done for 3D topological insulators, by applying the arguments of Ref.8 to the model (20). Situation described here is, in some sense, similar to the calculation of Z_2 invariants of topological insulators, where Brillouin zone is divided into two halves, related to each other by time-reversal symmetry.²² The difference is that here we deal with an effective field theory instead of microscopic model: by a suitable transformation, topological field theory is divided into two and a logic, familiar from the study of 3D topological insulators,⁸ is applied to each half.

Eq. (21) is consistent with general consideration of effective field theories of topological insulators.²³ It was shown in 23 that before specifying the properties of space-time, the lagrangian density of topological insulator is of BF type with two unknown coefficients

$$\Lambda_F(\varepsilon^{\mu\nu\rho\lambda}a_\mu\partial_\nu b_{\rho\lambda} + \varepsilon^{\mu\nu\rho\lambda}A_\mu\partial_\nu b_{\rho\lambda}) + C_F\varepsilon^{\mu\nu\rho\lambda}\partial_\mu a_\nu\partial_\rho A_\lambda$$

This theory assumes that collective excitations in the bulk of a topological insulator is given by neutral fermions, which couple to external fields by electric and magnetic dipole moments. It is reasonable to assume that collective excitations in topological crystalline insulators also can be described by this method.

VI. DISCUSSION

We have presented some arguments that the theory (21) might be an effective field theory for recently proposed topological crystalline insulators¹ in the case of C_4 symmetry. However the discussion has not been rigorous and there are some points that should be cleared. For example, transformation of momentum operators (7) was defined only in the continuous limit and we do not know what are the corresponding relations for a compact manifold. Such relations are necessary for a rigorous theory. We also did not explain why the model in $\tilde{}$ space is given by two copies of the model that was proposed as a topological field theory for time-reversal invariant topological insulators.⁸ One of the reasons for this choice was that this theory can easily explain Z_2 property and we did not know any other theories. Though it was not a priori stated that the theory must contain excitations with quarter flux quantum, we obtained that there are such excitations making quite reasonable propositions about the structure such a theory should possess. This last circumstance makes these propositions more plausible.

The other question is related to gapless surface excitations. It was shown in the Ref.8 how one can account for gapless surface excitations of 3D topological insulators in the context of BF theory. Electronic degrees of freedom on the surface are constructed using 2+1D bosonization scheme proposed in the Ref.24,25. In principle, some analogous procedure can be done in the case of fermions with gapless quadratic spectrum in the continuous limit, by reducing them first to fermions with linear spectrum. However it is more proper to study fermions with quadratic spectrum from the beginning in view of the following circumstance. In 2+1D in the continuum limit, internal energy of a single two-component fermion with gapless quadratic excitations is equal to internal energy of a boson with gapless quadratic excitations due to the identity

$$2 \int \frac{k^2 d^2k}{e^{\alpha k^2} + 1} = \int \frac{k^2 d^2k}{e^{\alpha k^2} - 1}$$

analogous to equivalence of internal energies of bosons and fermions in 1+1 D.²⁶ No such simple relation exists for 2+1D fermions and bosons with linear spectrum and bosonization of Dirac fermions with linear spectrum in 2+1D, as it was described in^{24,25}, is not fundamental.²⁷

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